

1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-
59950-41-3 | DTXSID40208664

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 42.9 days

Global applicability domain: Outside

Local applicability domain index: 3.14e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Acenaphthylene</div> <div>Measured: 4340</div> <div>Predicted: 36.6</div>	<div>Image not found</div> <div>9-Methylantracene</div> <div>Measured: 364000</div> <div>Predicted: 144</div>	<div>Image not found</div> <div>Acenaphthene</div> <div>Measured: 4610</div> <div>Predicted: 40.1</div>
<div>Image not found</div> <div>Tetralin</div> <div>Measured: 120</div> <div>Predicted: 12.2</div>	<div>Image not found</div> <div>Fluorene</div> <div>Measured: 6090</div> <div>Predicted: 42.2</div>	